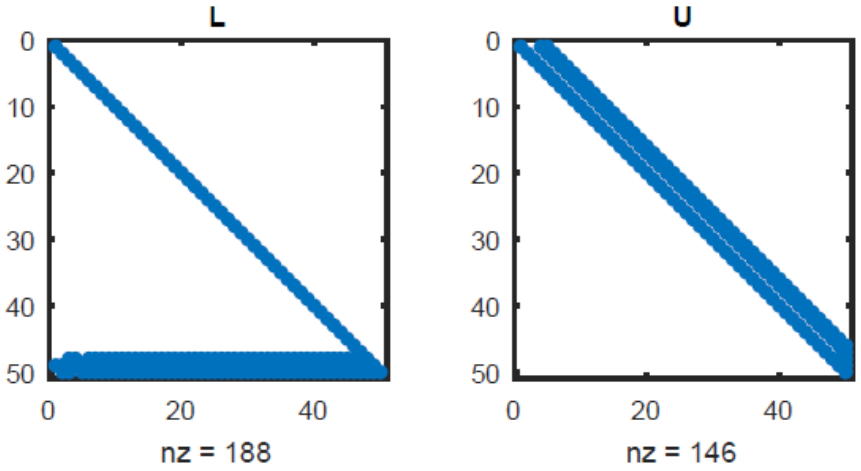
Chapter 8
Krylov Methods in Linear Algebra



Section 8.1
Sparsity and Structure

Methods for large matrices/systems

- We could also have called this chapter "Iterative methods"
- Depending on your computer, you may find it is difficult to store an $n \times n$ matrix where $n = 10^4$ 763 MB
- We need a way to compute at all for larger matrices
- We need ways to compute efficiently for larger matrices

$n = 10^5$: 74.5 GB

Sparse matrices

- One common case is when large matrices has many *structural zeros:* many elements are exactly zero
- In these *sparse matrices*, the fraction of nonzero entries may be quite small
- One uses much less storage to store only nonzero entries, and to do computations only for nonzero values
- Each nonzero entry $\{a_{ij}\}$ in the matrix ***A*** can be stored as a triple (i, j, a_{ij})
- One then has to write code that can correctly use only the nonzero entries; we will not do this
- But, we will exploit Matlab's capabilities in this area

Example: large adjacency matrix

Example 8.1.1

A is an adjacency matrix for web pages making about Roswell, NM, and how they link to each other.

```
load roswelladj   % get from the book's website
a = whos('A')
```

```
a =
          name: 'A'
          size: [2790 2790]
         bytes: 158120
         class: 'double'
        global: 0
        sparse: 1
       complex: 0
       nesting: [1x1 struct]
    persistent: 0
```

- It's large
- The elements are double precision
- It's sparse!
- Real valued

Example: large adjacency matrix

Example 8.1.1

Each nonzero entry in A corresponds to an edge; we can compute fraction of nonzeros: call that the density

```
sz = size(A);  n = sz(1);
density = nnz(A) / prod(sz)
```

```
density =
    0.0011
```

`size` returns the number of rows and columns

`nnz` returns the number of nonzero elements

Sparse!

```
F = full(A);
f = whos('F');
a.bytes/f.bytes
```

`full` creates the full matrix storage version

```
ans =
    0.0025
```

Compare storage of sparse vs full matrix versions

How about computation time?

Example: large adjacency matrix

Example 8.1.1

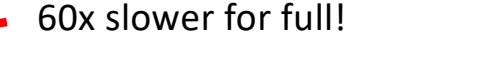
Computation time for sparse vs full? Sparse uses only nonzeros

```
x = randn(n,1);
tic, for i = 1:200, A*x; end
sparse_time = toc
```

```
sparse_time =
    0.0107
```

```
tic, for i = 1:200, F*x; end
dense_time = toc
```

```
dense_time =
    0.6207
```



`tic and toc` for timing

Matrix vector products first

Create random vector, repeat 200x for timing

Sparse first, then full

60x slower for full!

Example: large adjacency matrix

Example 8.1.1

Computation time for row operations can be slower: Matlab's sparse storage is column oriented

```
v = A(:,1000);
tic, for i = 1:n, A(:,i)=v; end
column_time = toc
r = v';
tic, for i = 1:n, A(i,:)=r; end
row_time = toc
```

Column oriented

Row oriented

```
column_time =
    0.0079
row_time =
    0.0630
```

8x slower for rows

[Example 8.1.1]

Matrix fill-in

- Arithmetic operations *,+,-,^ can exploit sparsity
- But, matrix operations can reduce the sparsity: *matrix fill-in*

Example 8.1.2

Here is the buckyball adjacency matrix again.

```
[A,v] = bucky;
```

The number of vertex pairs on a soccer ball connected by a path of length $k > 1$ grows with k, as can be seen here for $k = 3$.

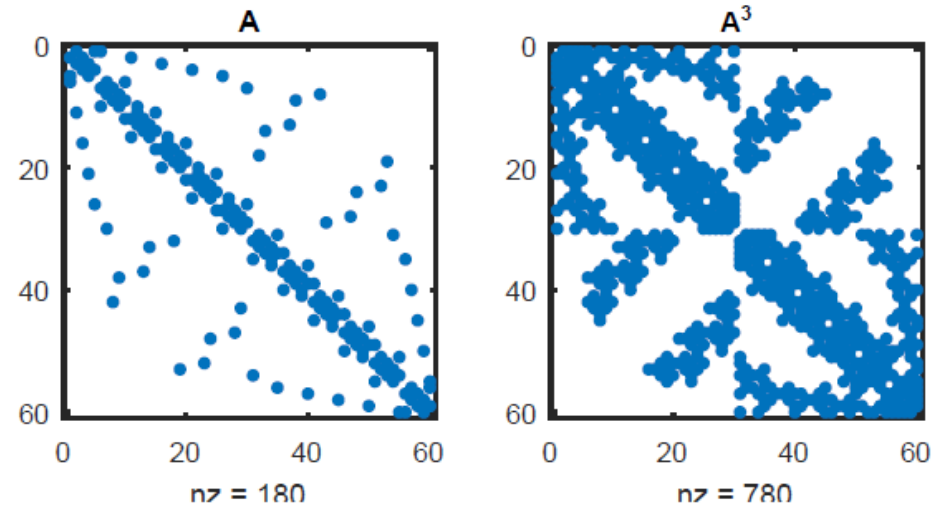
```
subplot(1,2,1), spy(A)
subplot(1,2,2), spy(A^3)
```

The `spy` command plots nonzero elements and gives the number of nonzeros…

Matrix fill-in

[Example 8.1.2]

Example 8.1.2

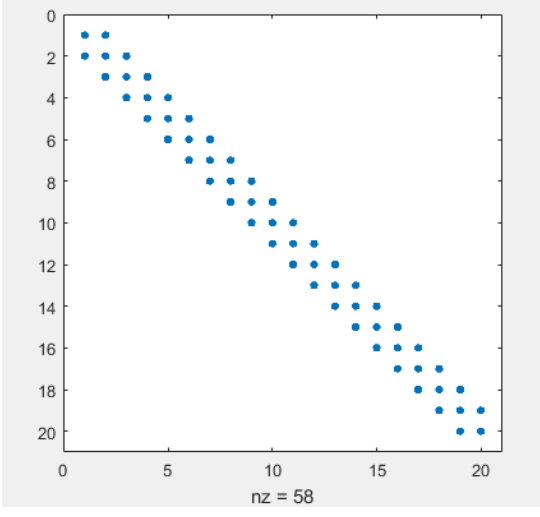


The number of nonzeros increased by more than 4x

Banded matrices

- This is an important class of matrices that comes up in applications
- The simplest is the diagonal matrix: bandwidth 1
- Another is tridiagonal, with main diagonal, as well as one superdiagonal and one subdiagonal: bandwidth is 3
- More generally, if p nonzero superdiagonals, and q nozero subdiagonals, then bandwidth is p+q+1

```
>> n=20;
>> v = ones(n,1);
>> d = [-v 2*v -0.5*v];
>> pos = [-1 0 1];
>> A = spdiags(d,pos,n,n);
>> spy(A)
>>
```



Example: solving a banded system

Example 8.1.3

```
n = 50;
d = [ n*ones(n,1), ones(n,1), -(1:n)'];   % diagonal entries
pos = [-3 0 1];                           % which diagonals
A = spdiags(d,pos,n,n);
full( A(1:7,1:7) )
```

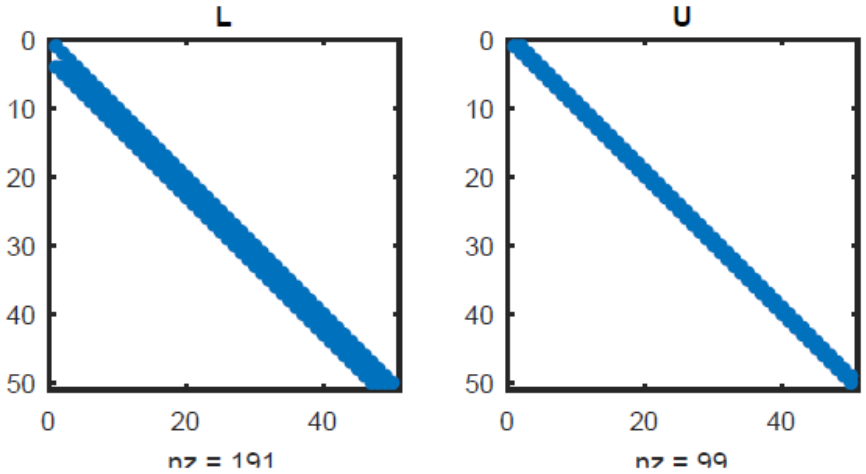
```
ans =
     1    -2     0     0     0     0     0
     0     1    -3     0     0     0     0
     0     0     1    -4     0     0     0
    50     0     0     1    -5     0     0
     0    50     0     0     1    -6     0
     0     0    50     0     0     1    -7
     0     0     0    50     0     0     1
```

- Sparse tridiagonal matrix created
- Matlab trims the size of the vectors put into the diagonals
- Full version displayed
- Solving a system?

Example: solving a banded system

Example 8.1.3

```
[L,U] = lufact(A);
subplot(1,2,1), spy(L), title('L')
subplot(1,2,2), spy(U), title('U')
```



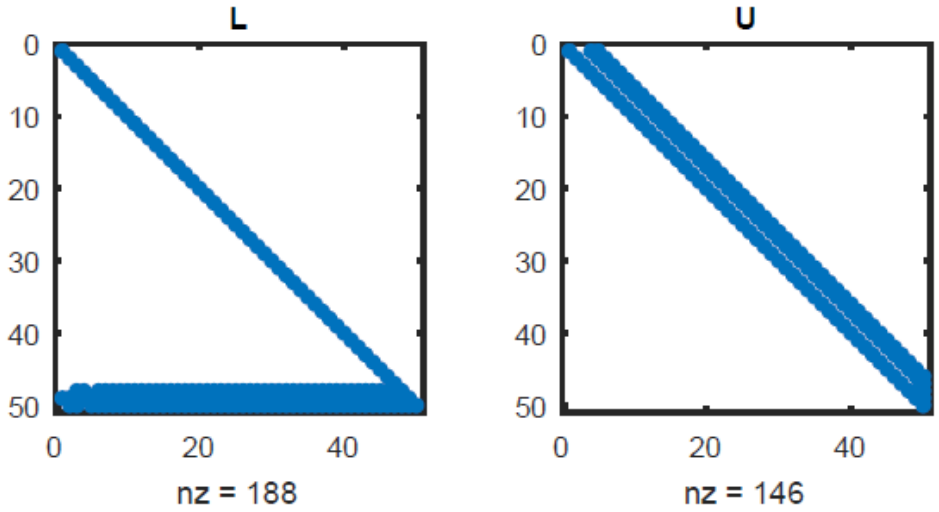
- No pivoting here
- Small bandwidth preserved

Example: solving a banded system

Example 8.1.3

```
[L,U,P] = lu(A);
subplot(1,2,1), spy(L), title('L')
subplot(1,2,2), spy(U), title('U')
```

[Example 8.1.3]



- Pivoting used here
- Bandwidth grows a little in U, but a lot in L to roughly n/2

Linear systems and eigenvalues

- Say one starts with a sparse matrix ***A*** and compatible right-hand-side ***b***
- In Matlab, A\b will automatically try a sparse-aware form of Cholesky or pivoted LU factorization Julia: multiple dispatch
- This approach could beat the O(n^3) cost for the general case with a full matrix, but this depends on the sparsity pattern of ***A***
- For a very large ***A***, it is unlikely that one would compute all of the eigenvalues and eigenvectors of ***A,*** that is, one would typically not use `eig` for very large matrices Julia: eigen, eigvals, eigs
- For very large ***A***, one would use `eigs` (Sec 8.4) to find the a selected number of eigenvalues, often the largest or those nearest a selected complex number (the s at the end indicates sparse; there is a similar `svds` command) Julia: svd, svdvals, svds

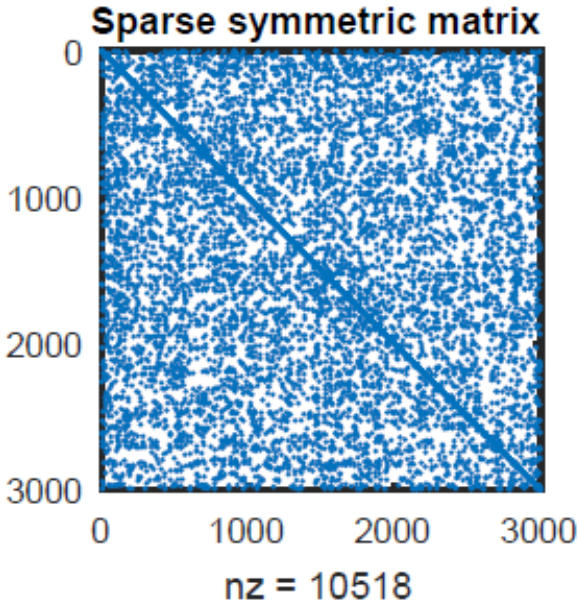
Example: sparse matrix eigenvalues

Example 8.1.4

The sprandsym command generates a random sparse matrix with prescribed eigenvalues.

```
n = 3000;
density = 1.23e-3;
lambda = 1./(1:n);
A = sprandsym(n,density,lambda);
spy(A)
eigs(A,5)     % largest magnitude
```

```
ans =
    1.0000
    0.5000
    0.3333
    0.2500
    0.2000
```



Example: sparse matrix eigenvalues

Example 8.1.4

```
eigs(A,5,0)  % closest to zero
```

```
ans =
   1.0e-03 *
    0.3338
    0.3337
    0.3336
    0.3334
    0.3333
```

- Predicting order of FlOps is difficult without info re ***A***
- But sparse calculation is often faster

[Example 8.1.4]

```
x = 1./(1:n)';  b = A*x;
tic, sparse_err = norm(x - A\b), sparse_time = toc
```

```
sparse_err =
   2.1074e-14
sparse_time =
    0.0110
```

```
A = full(A);
tic, dense_err = norm(x - A\b), dense_time = toc
```

```
dense_err =
   7.2768e-14
dense_time =
    0.2792
```

Section 8.2
Power Iteration

Google Pagerank algorithm

Example: repeated matrix multiplication

Let's use that fast matrix-vector multiplication

Example 8.2.1

```
A = magic(5)/65;
x = randn(5,1)
```

```
x =
    1.7491
    0.1326
    0.3252
   -0.7938
    0.3149
```

```
y = A*x
```

```
y =
    0.4864
    0.5707
    0.0473
    0.1467
    0.4770
```

```
z = A*y
```

```
z =
    0.4668
    0.3701
    0.2987
    0.2634
    0.3291
```

- Nothing to good happening yet
- Now try more factors of ***A***

Example: repeated matrix multiplication

Example 8.2.1

```
for j = 1:8,   x = A*x;   end
[x,A*x]
```

```
ans =
    0.3457    0.3457
    0.3457    0.3456
    0.3455    0.3456
    0.3455    0.3456
    0.3456    0.3456
```

- After 8 times, we are getting $\boldsymbol{Ax} \approx \boldsymbol{x}$
- But this seems to happen lots of initial vectors

```
x = randn(5,1)
for j = 1:8,   x = A*x;   end
[x,A*x]
```

```
x =
   -0.5273
    0.9323
    1.1647
   -2.0457
   -0.6444
ans =
   -0.2240   -0.2241
   -0.2239   -0.2241
   -0.2239   -0.2241
   -0.2242   -0.2241
   -0.2243   -0.2240
```

Example: repeated matrix multiplication

Example 8.2.1

- Using eig, we find that the eigenvalues are 1, ±0.327, ±0.202
- It turns out that we would be right to think that the process at left is converging to $\boldsymbol{Ax} = \lambda \boldsymbol{x}$ with $\lambda = 1$
- It turns out that this process converges to the largest eigenvalue and its associated eigen~~value~~ vector
- Why?

[Example 8.2.1]

```
x = randn(5,1)
for j = 1:8,   x = A*x;   end
[x,A*x]
```

```
x =
   -0.5273
    0.9323
    1.1647
   -2.0457
   -0.6444
ans =
   -0.2240   -0.2241
   -0.2239   -0.2241
   -0.2239   -0.2241
   -0.2242   -0.2241
   -0.2243   -0.2240
```

Dominant eigenvalue

- Suppose that we have an $n \times n$ diagonalizable matrix $\boldsymbol{A}$
- The eigenvalues are $\lambda_1, \lambda_2, \ldots, \lambda_n$ with associated eigenvectors $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n$
- Suppose also that

$$|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_n|.$$

- λ_1 is the dominant eigenvalue
- The $\boldsymbol{v}_k$ are an LI set, so we can express the general initial vector as a linear combo of them:

$$\boldsymbol{x} = c_1\boldsymbol{v}_1 + c_2\boldsymbol{v}_2 + \cdots + c_n\boldsymbol{v}_n.$$

- We know that $\boldsymbol{A}\boldsymbol{v}_k = \lambda_k\boldsymbol{v}_k$; use that with repeated mult by $\boldsymbol{A}$

Dominant eigenvalue

- First,

$$\begin{aligned} \boldsymbol{A}\boldsymbol{x} &= c_1\boldsymbol{A}\boldsymbol{v}_1 + c_2\boldsymbol{A}\boldsymbol{v}_2 + \cdots + c_n\boldsymbol{A}\boldsymbol{v}_n \\ &= c_1\lambda_1\boldsymbol{v}_1 + c_2\lambda_2\boldsymbol{v}_2 + \cdots + c_n\lambda_n\boldsymbol{v}_n. \end{aligned}$$

- Now use this repeatedly, factor out dominant eigenvalue

$$\begin{aligned} \boldsymbol{A}^k\boldsymbol{x} &= \lambda_1^k c_1\boldsymbol{v}_1 + \lambda_2^k c_2\boldsymbol{v}_2 + \cdots + \lambda_n^k c_n\boldsymbol{v}_n \\ &= \lambda_1^k \left[c_1\boldsymbol{v}_1 + \left(\frac{\lambda_2}{\lambda_1}\right)^k c_2\boldsymbol{v}_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^k c_n\boldsymbol{v}_n \right]. \end{aligned}$$

- Does the left side approach $c_1\boldsymbol{v}_1$? How fast?

Dominant eigenvalue

- Rewrite the equation a bit: divide by λ_1^k, and subtract $c_1 \boldsymbol{v}_1$ from both sides to get

$$\frac{\boldsymbol{A}^k \boldsymbol{x}}{\lambda_1^k} - c_1 \boldsymbol{v}_1 = \left(\frac{\lambda_2}{\lambda_1}\right)^k c_2 \boldsymbol{v}_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^k c_n \boldsymbol{v}_n$$

- Now take a norm of both sides, and use the triangle inequality:

$$\left\| \frac{\boldsymbol{A}^k \boldsymbol{x}}{\lambda_1^k} - c_1 \boldsymbol{v}_1 \right\| \leq |c_2| \cdot \left|\frac{\lambda_2}{\lambda_1}\right|^k \|\boldsymbol{v}_2\| + \cdots + |c_n| \cdot \left|\frac{\lambda_n}{\lambda_1}\right|^k \|\boldsymbol{v}_n\| \to 0 \text{ as } k \to \infty.$$

- The right side tends to zero because the ratios of eigenvalues are all less than one: $A^k x$ becomes almost parallel to dominant eigenvector
- We need $c_1 \neq 0$, essentially guaranteed with random initial vector
- Important to think of this as repeated matrix vector multiplication

Power iteration

- We do repeated matrix-vector multiplication
- To make a more practical method, we also renormalize the vector with it's largest element each iteration
- Let $|y_{k,m}| = ||y_k||_\infty$ (m is mth component)
- Note $||x_{k+1}||_\infty = 1$

Power iteration algorithm:

1. Choose x_1.
2. For $k = 1, 2, \ldots$

$$y_k = Ax_k,$$
$$\alpha_k = \frac{1}{y_{k,m}}, \text{ where } |y_{k,m}| = \|y_k\|_\infty,$$
$$x_{k+1} = \alpha_k y_k.$$

Note that

$$x_2 = \alpha_1 A x_1$$

$$x_3 = \alpha_2 A x_2 = \alpha_1 \alpha_2 A^2 x_1$$

$$\vdots$$

$$\boxed{x_{k+1} = \alpha_1 \alpha_2 \cdots \alpha_k A^k x_1}$$

Since $y_k = A x_k$, if $A x_k \approx \lambda_1 x_k$,

then $y_k \approx \lambda_1 x_k$, so $y_{k,m} \approx \lambda_1 x_{k,m}$.

($y_{k,m}$: largest in abs. val.)

Thus, $\boxed{\dfrac{y_{k,m}}{x_{k,m}} \approx \lambda_1}$. In fact,

$$\frac{y_{k,m}}{x_{k,m}} = \frac{(Ax_k)_m}{(x_k)_m} = \frac{\alpha_1 \cdots \alpha_{k-1} (A^k x_1)_m}{\alpha_1 \cdots \alpha_{k-1} (A^{k-1} x_1)_m} = \frac{(A^k x_1)_m}{(A^{k-1} x_1)_m}$$

$$= \frac{\lambda_1^k \left[c_1 v_1 + \left(\frac{\lambda_2}{\lambda_1}\right)^k c_2 v_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^k c_n v_n \right]_m}{\lambda_1^{k-1} \left[c_1 v_1 + \left(\frac{\lambda_2}{\lambda_1}\right)^{k-1} c_2 v_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^{k-1} c_n v_n \right]_m}$$

Let $r_j = \dfrac{\lambda_j}{\lambda_1}$, for $j = 2, \ldots, n$.

Then $|r_j| < 1$, for $j = 2, \ldots, n$, so

$$\frac{y_{k,m}}{x_{k,m}} = \lambda_1 \frac{\left[c_1 v_1 + r_2^k c_2 v_2 + \cdots + r_n^k c_n v_n\right]_m}{\left[c_1 v_1 + r_2^{k-1} c_2 v_2 + \cdots + r_n^{k-1} c_n v_n\right]_m}$$

$$\xrightarrow[(\text{as } k \to \infty)]{} \lambda_1 \frac{[c_1 v_1]_m}{[c_1 v_1]_m} = \lambda_1 .$$

We let $\gamma_k = \dfrac{y_{k,m}}{x_{k,m}}$. Then

$$\boxed{\gamma_k \to \lambda_1 \quad \text{as} \quad k \to \infty .}$$

Moreover, it can be shown that

$$\boxed{\frac{\gamma_{k+1} - \lambda_1}{\gamma_k - \lambda_1} \longrightarrow \frac{\lambda_2}{\lambda_1} \quad \text{as} \quad k \to \infty}$$

which tells us that $\gamma_k \to \lambda_1$ at a linear rate.

Dominant eigenvalue

- What about the eigenvalue?
- *k*th approximation is

$$\gamma_k = \frac{y_{k,m}}{x_{k,m}} = \lambda_1 \frac{1 + r_2^{k+1} b_2 + \cdots + r_n^{k+1} b_n}{1 + r_2^k b_2 + \cdots + r_n^k b_n},$$

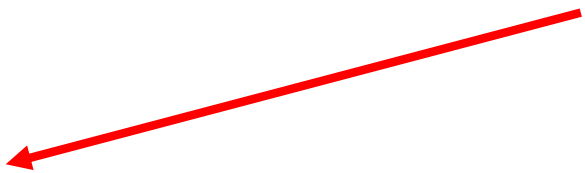
where $r_j = \lambda_j / \lambda_1$ and the b_j are constants.

$r_j < 1$

- With our ordering, $r_j < 1$, and we have convergence to the dominant eigenvalue as $k \to \infty$
- Function `poweriter` implements this in Matlab

Function `poweriter`

```
1  function [gamma,x] = poweriter(A,numiter)
2  % POWERITER   Power iteration for the dominant eigenvalue.
3  % Input:
4  %   A          square matrix
5  %   numiter    number of iterations
6  % Output:
7  %   gamma      sequence of eigenvalue approximations (vector)
8  %   x          final eigenvector approximation
9
10 n = length(A);
11 x = randn(n,1);
12 x = x/norm(x,inf);
13 for k = 1:numiter
14   y = A*x;
15   [normy,m] = max(abs(y));
16   gamma(k) = y(m)/x(m);
17   x = y/y(m);
18 end
```



- `max` returns max value and location in vector
- Sparsity used automatically

Convergence of power iteration

- Return to *k*th approximation:

$$\gamma_k = \frac{y_{k,m}}{x_{k,m}} = \lambda_1 \frac{1 + r_2^{k+1} b_2 + \cdots + r_n^{k+1} b_n}{1 + r_2^k b_2 + \cdots + r_n^k b_n},$$

where $r_j = \lambda_j / \lambda_1$ and the b_j are constants.

- Consider the denominator:

$$\begin{aligned} r_2^k b_2 + \cdots + r_n^k b_n &= r_2^k \left[b_2 + \left(\frac{r_3}{r_2} \right)^k b_3 + \cdots + \left(\frac{r_n}{r_2} \right)^k b_n \right] \\ &= r_2^k \left[b_2 + \left(\frac{\lambda_3}{\lambda_2} \right)^k b_3 + \cdots + \left(\frac{\lambda_n}{\lambda_2} \right)^k b_n \right]. \end{aligned}$$

- For simplicity, assume that $|\lambda_2| > |\lambda_3| \geq \cdots \geq |\lambda_n|$.

Convergence of power iteration

- With this assumption all of the ratios $\left(\frac{r_j}{r_2}\right)^k \to 0$ for $k \to \infty$, so that the term approaches just the leading term, $b_2 r_2^k$, for large k
- With the simpler denominator, it is relatively easy to use a geometric series for it
- Using that in the eigenvalue approximation gives

$$\gamma_k \to \lambda_1 \left(1 + b_2 r_2^{k+1}\right) \left(1 - b_2 r_2^k + O(r_2^{2k})\right),$$
$$\gamma_k - \lambda_1 \to \lambda_1 b_2 (r_2 - 1) r_2^k.$$

- The next term has $\gamma_{k+1} - \lambda_1 \to \lambda_1 b_2 (r_2 - 1) r_2^{k+1}$
- Dividing the last two expressions tells us what happens each iteration…

Convergence of power iteration

- We find that the ratio is

$$\frac{\gamma_{k+1} - \lambda_1}{\gamma_k - \lambda_1} \to r_2 = \frac{\lambda_2}{\lambda_1} \quad \text{as } k \to \infty.$$

- The new approximation is roughly a factor of r_2 closer than the old one
- This is linear convergence: the error drops by a constant factor each time
- It is usually true once one has a done a few iterations, so that the computed values start to come from "large k"
- Thinking of taking this limit for a (potentially) large number of iterations is what we mean when we say:

The error in the eigenvalue estimates γ_k of power iteration is reduced asymptotically by a constant factor λ_2/λ_1 on each iteration.

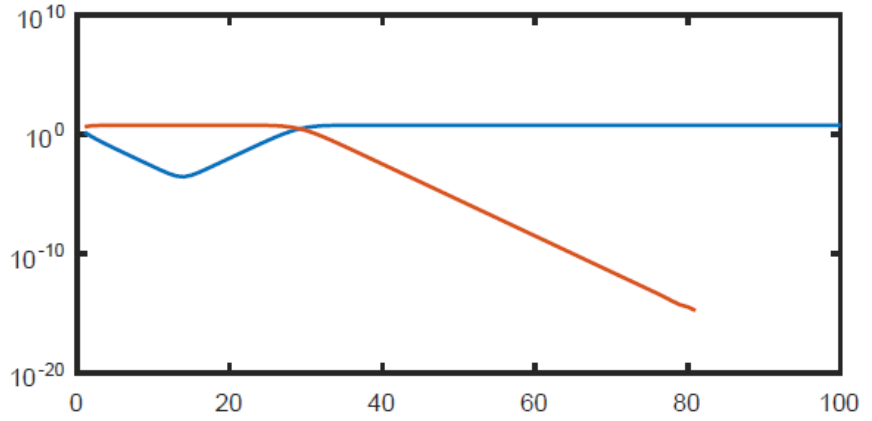
Example: convergence

[Example 8.2.2]

Example 8.2.2

```
A= [ 6 3 3; 1 10 1; 2 5 5];
[V,D] = eig(A);
x = [2;-1;2]+1e-8;
for n = 1:100
    y = A*x;
    [~,m] = max(abs(y));
    gamma(n) = y(m)/x(m);
    x = y/y(m);
end
semilogy(abs(gamma-6))
hold on, semilogy(abs(gamma-12))
```

- How fast do iterates gamma converge to eigenvalues?
- Blue: $\lambda_2 = 6$; red: $\lambda_1 = 12$
- Linear convergence to λ_1



Convergence of power iteration

- This is not a practical implementation
- We will continue to improved methods

Section 8.3
Inverse Iteration

Inverse iteration

- Power iteration only finds the dominant eigenvalue
- We can extend power iteration to find other eigenvalues
- The idea is to use some simple linear algebra results to change the relative sizes of the eigenvalues

Inverse iteration

- Here are those linear algebra results

Theorem 8.3.1

Let $\boldsymbol{A}$ be an $n \times n$ matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$ (possibly with repeats), and let s be a complex scalar. Then:

1. The eigenvalues of the matrix $\boldsymbol{A} - s\boldsymbol{I}$ are $\lambda_1 - s, \ldots, \lambda_n - s$.
2. If s is not an eigenvalue of $\boldsymbol{A}$, the eigenvalues of the matrix $(\boldsymbol{A} - s\boldsymbol{I})^{-1}$ are $(\lambda_1 - s)^{-1}, \ldots, (\lambda_n - s)^{-1}$.
3. The eigenvectors associated with the eigenvalues in the first two parts are the same as those of $\boldsymbol{A}$.

Inverse iteration

- Great options for moving around eigenvalues, if true
- Consider item 1: start with $\boldsymbol{Av} = \lambda \boldsymbol{v}$; subtract $s\boldsymbol{Iv}$ from both sides

$$\boldsymbol{Av} - s\boldsymbol{Iv} = \lambda \boldsymbol{v} - s\boldsymbol{Iv} \rightarrow$$
$$(\boldsymbol{A} - s\boldsymbol{I})\boldsymbol{v} = (\lambda - s)\boldsymbol{v}$$

- We have that a matrix times a vector gives a scalar times the same vector, as in part 1: proven.
- For part 2, we assumed that $s \neq \lambda_k$, so $\boldsymbol{A} - s\boldsymbol{I}$ is non-singular, then straightforward rearrangement gives

$$(\boldsymbol{A} - s\boldsymbol{I})^{-1}\boldsymbol{v} = (\lambda_k - s)^{-1}\boldsymbol{v}$$

- This proves that item 2 is true.
- Item 3 follows too.

Inverse iteration

- Consider item 2 with $s = 0$: start with $\boldsymbol{A}$ having a *smallest* eigenvalue:

$$|\lambda_n| \geq |\lambda_{n-1}| \geq \cdots > |\lambda_1|.$$

- Then

$$|\lambda_1^{-1}| > |\lambda_2^{-1}| \geq \cdots \geq |\lambda_n^{-1}|,$$

so that the reciprocal of the smallest eigenvalue is now the dominant one

- We can use power iteration to find the reciprocal value, and thus approximate the smallest eigenvalue (the one closest to zero)
- This is *inverse iteration*
- The convergence rate is linear again, with rate $\dfrac{\lambda_2^{-1}}{\lambda_1^{-1}} = \dfrac{\lambda_1}{\lambda_2}.$

Shifted inverse iteration

- Consider $s \neq 0$: order eigenvalues of $\boldsymbol{A} - s\boldsymbol{I}$ with distance from s

$$|\lambda_n - s| \geq \cdots \geq |\lambda_2 - s| > |\lambda_1 - s|,$$

- Then

$$|\lambda_1 - s|^{-1} > |\lambda_2 - s|^{-1} \geq \cdots \geq |\lambda_n - s|^{-1}.$$

- We can use power iteration to find the first reciprocal value, and thus approximate the eigenvalue closest to s
- This is *shifted inverse iteration*
- Power iteration on $(\boldsymbol{A} - s\boldsymbol{I})^{-1}$ converges to $(\lambda_1 - s)^{-1}$ provided that λ_1 is closest to s

Shifted inverse iteration

- There is a new computational wrinkle here
- We want to find: $y_k = (A - sI)^{-1} x_k.$ for a sequence of k values
- However, we do NOT want to compute $(A - sI)^{-1}$ to do it!
- Instead, we could write what is needed as

$$\text{Solve } (A - sI)y_k = x_k \text{ for } y_k.$$

- The solve is the computational version of the inverse, but is faster !!!

Shifted inverse iteration

$y = (A - sI) \backslash x$

C will factor $A - sI$ each time

- We need

$$\text{Solve } (\boldsymbol{A} - s\boldsymbol{I})\boldsymbol{y}_k = \boldsymbol{x}_k \text{ for } \boldsymbol{y}_k.$$

- To begin with, we use PLU factorization, and live with any fill-in that may result for sparse matrices
- Function 8.3.1 does inverse iteration
- Note that the iteration is for $\beta_k = (\gamma_k - s)^{-1}$; the approximation to the original eigenvalue is $\gamma_k = s + \beta_k^{-1}$

Function `inviter`

Function 8.3.1 (inviter) Shifted inverse iteration for the closest eigenvalue.

```
function [gamma,x] = inviter(A,s,numiter)
% INVITER   Shifted inverse iteration for the closest eigenvalue.
% Input:
%   A          square matrix
%   s          value close to targeted eigenvalue (complex scalar)
%   numiter    number of iterations
% Output:
%   gamma      sequence of eigenvalue approximations (vector)
%   x          final eigenvector approximation

n = length(A);
x = randn(n,1);
x = x/norm(x,inf);
B = A - s*eye(n);
[L,U] = lu(B);
for k = 1:numiter
  y = U \ (L\x);
  [normy,m] = max(abs(y));
  gamma(k) = x(m)/y(m) + s;
  x = y/y(m);
end
```

- Random x ensures some component in eigenvector direction
- Should be `s*speye(n)` here

Example: inverse iteration

Example 8.3.1

```
lambda = [1 -0.75 0.6 -0.4 0];
A = triu(ones(5),1) + diag(lambda);
format long

[gamma,x] = inviter(A,0.7,30);
eigval = gamma(end)
```

```
eigval =
   0.599999999999998
```

- Create a 5×5 matrix with known eigenvalues
- Use $s = 0.7$ and do 30 iterations
- Convergence is to closest eigenvalue with value 0.6

Example: inverse iteration

Example 8.3.1

```
observed_rate = err(26)/err(25)

observed_rate =
  -0.327983951855567

theoretical_rate = (lambda(3)-0.7) / (lambda(1)-0.7)

theoretical_rate =
  -0.333333333333333
```

- We could also compute the ratio $(\gamma_{k+1} - s)/(\gamma_k - s)$ in Matlab using s=0.7 and

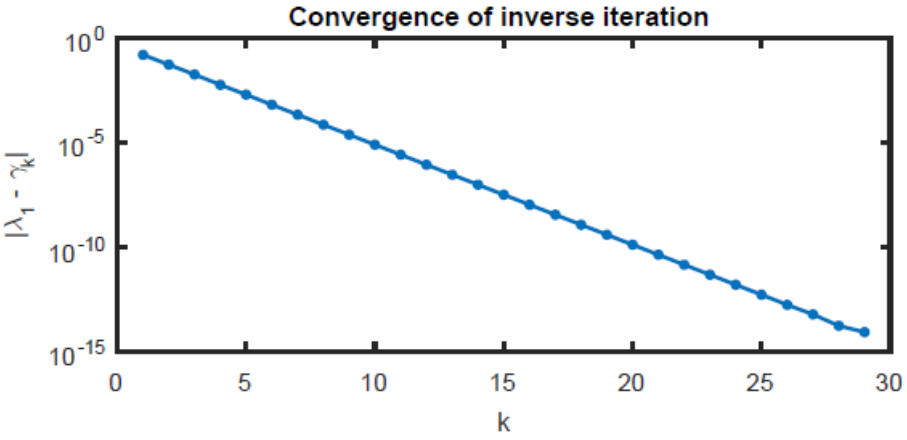
```
seq_of rate = (gamma(2:end)-s)./(gamma(1:end-1)-2)
```

and see that the sequence of ratios approaches 1/3

Example: inverse iteration

Example 8.3.1

```
err = eigval - gamma;
semilogy(abs(err),'.-')
```



- Convergence rate is linear: drops by constant factor of about 0.33 each time
- How do we know this?

[Example 8.3.1]

Dynamic shifting

- In our last example, we left s as a single value throughout the iteration
- This works reasonably well, but one can do better
- This time, let $s = \gamma_k$ when we compute γ_{k+1}
- So, we are adjusting s on the fly
- How well does it work?

Example: inverse iteration

Example 8.3.2

```
lambda = [1 -0.75 0.6 -0.4 0];
A = triu(ones(5),1) + diag(lambda);
format long
I = eye(5);  s = 0.7;
x = ones(5,1);
y = (A-s*I)\x;  gamma = x(1)/y(1) + s
```

```
gamma =
   0.703481392557023
```

```
s = gamma;
x = y/y(1);
y = (A-s*I)\x;  gamma = x(1)/y(1) + s
```

```
gamma =
   0.561276140617300
```

- Same 5×5 matrix as previous example
- Use $s = 0.7$ and do 1 iteration
- Change s to γ and repeat
- Doesn't look too good yet, but…

Example: inverse iteration

Example 8.3.2

```
for k = 1:4
    s = gamma;   x = y/y(1);
    y = (A-s*I)\x;   gamma = x(1)/y(1) + s
end
```

```
gamma =
   0.596431288475387
gamma =
   0.599971709182010
gamma =
   0.599999997855635
gamma =
   0.600000000000000
```

[Example 8.3.2]

- Now repeat the process a few times
- Boom!
- Convergence is very rapid: roughly double the number of digits each time
- This is *quadratic convergence*
- Like Newton's method near a root

Dynamic shifting

- There is a price for this increased rate of convergence
- Before, with constant shift, we could factor $\boldsymbol{A} - s\boldsymbol{I}$ once, and each iterate is faster, but there can be many more
- With dynamic shifting, we need to factor $\boldsymbol{A} - s_k\boldsymbol{I}$ for each iteration but there may be many fewer iterations
- For our examples, 30 iterates for constant shift, only 6 with dynamic shift
- In many cases it pays off to dynamically shift.

Section 8.4
Krylov Subspaces

Krylov subspaces

- Say we start with a seed vector $\boldsymbol{u}$
- If we repeatedly multiply by a matrix $\boldsymbol{A}$, we can keep all of the products, and try to use that set as a basis for approximating answers.
- Thus, we are creating the set $\boldsymbol{u}, \boldsymbol{Au}, \boldsymbol{A^2u}, \ldots$
- In the power or inverse iterations we only kept the latest on each time
- We get the $n \times m$ *Krylov matrix* if the columns are $\boldsymbol{u}, \boldsymbol{Au}, \boldsymbol{A^2u}, \ldots$

$$K_m = \begin{bmatrix} u & Au & A^2u & \cdots & A^{m-1}u \end{bmatrix}$$

Krylov subspaces

- The columns of the $n \times m$ Krylov matrix are important

$$K_m = \begin{bmatrix} u & Au & A^2u & \cdots & A^{m-1}u \end{bmatrix}$$

- The columns form the mth Krylov subspace $\mathcal{K}_m$ of $\mathbb{C}^n$
- Each column is n long, but there are only m columns
- We want to approximate answers from this subspace; said another way, we want to find answers that are a linear combo of the columns
- The dimension of $\mathcal{K}_m$ is the same as the rank of K_m, which is often m but may be smaller

Properties

- Generating columns of Krylov matrix is relatively easy for sparse $\boldsymbol{A}$

$$\boldsymbol{K}_m = \begin{bmatrix} \boldsymbol{u} & \boldsymbol{A}\boldsymbol{u} & \boldsymbol{A}^2\boldsymbol{u} & \cdots & \boldsymbol{A}^{m-1}\boldsymbol{u} \end{bmatrix}$$

- And, there are some nice properties…

Lemma 8.4.1

Suppose $\boldsymbol{A}$ is $n \times n$, $0 < m < n$, and a vector $\boldsymbol{u}$ is used to generate Krylov subspaces. If $\boldsymbol{x} \in \mathcal{K}_m$, then the following hold:

1. $\boldsymbol{x} = \boldsymbol{K}_m \boldsymbol{z}$ for some $\boldsymbol{z} \in \mathbb{C}^m$
2. $\boldsymbol{x} \in \mathcal{K}_{m+1}$
3. $\boldsymbol{A}\boldsymbol{x} \in \mathcal{K}_{m+1}$

Properties

- Part 1 simply says that if $\boldsymbol{x} \in \mathcal{K}_m$, then for some coefficients $c_1, c_2, \ldots, c_m$, $\boldsymbol{x}$ can be written as

$$x = c_1 u + c_2 A u + \cdots + c_m A^{m-1} u.$$

- Then, let $z = [c_1\ c_2\ \ldots\ c_m]^T$, and recall that

$$K_m = \begin{bmatrix} u & Au & A^2u & \cdots & A^{m-1}u \end{bmatrix}$$

- For Part 3, just multiply the first equation by A, and one has

$$Ax = c_1 Au + c_2 A^2 u + \cdots + c_m A^m u \in \mathcal{K}_{m+1}.$$

Reducing dimension and solving linear systems

- Consider the linear system $\boldsymbol{A}x = \boldsymbol{b}$ for $n \times n$ nonsingular $\boldsymbol{A}$
- The original idea for using Krylov subspaces was to create a space with n basis vectors, $\mathcal{K}_n$
- This could come with a predetermined number of steps, making it a direct method ($m = n$ here for multiplications by $\boldsymbol{A}$)

$$K_m = \begin{bmatrix} u & Au & A^2u & \cdots & A^{m-1}u \end{bmatrix}$$

- However, the columns of K_m effectively come from power method
- The columns are converging to the dominant eigenvector
- This makes the *direct method* with $m = n$ ill-conditioned and impractical

Reducing dimension and solving linear systems

- An alternative view is to say that most of the approximation or information is in the first few columns; the farther out columns are nearly dependent
- Why not stop early and perhaps get a good approximation with only $m < n$ basis vectors, that is, $\mathcal{K}_m$
- The problem changes then to one where we don't know in advance when to stop: it becomes an iterative method.
- Also, we need to get the best answer for the system $\boldsymbol{A}x = \boldsymbol{b}$ with n unknowns: this suggests a minimization of the error:

$$\min_{\boldsymbol{x}\in\mathcal{K}_m} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\| = \min_{\boldsymbol{z}\in\mathbb{C}^m} \|\boldsymbol{A}(\boldsymbol{K}_m\boldsymbol{z}) - \boldsymbol{b}\| = \min_{\boldsymbol{z}\in\mathbb{C}^m} \|(\boldsymbol{A}\boldsymbol{K}_m)\boldsymbol{z} - \boldsymbol{b}\|.$$

Reducing dimension and solving linear systems

- For the linear system $\boldsymbol{Ax = b}$, the natural choice to start the Krylov iteration is $\boldsymbol{u = b}$

$$K_m = \begin{bmatrix} u & Au & A^2u & \cdots & A^{m-1}u \end{bmatrix}$$

- We do adjust the size of each column with a normalization to prevent wildly different sizes of the elements
- Let's do an example

Example: Krylov iteration

Example 8.4.1

```
% Create a triangular matrix with
% known eigenvalues and a random vector b
lambda = 10 + (1:100) ;
A = diag( lambda ) + triu( rand(100),1 );
b = rand(100 ,1) ;

% Next we build up the first thirty Krylov
% matrices iteratively, using renormalization
% after each matrix-vector multiplication.
Km = b;
for m = 1:29
    v = A*Km(:,m);
    Km(:,m+1) = v/norm (v);
end
```

- mth column of K_m created each time
- Normalize the column and append it

Example: Krylov iteration

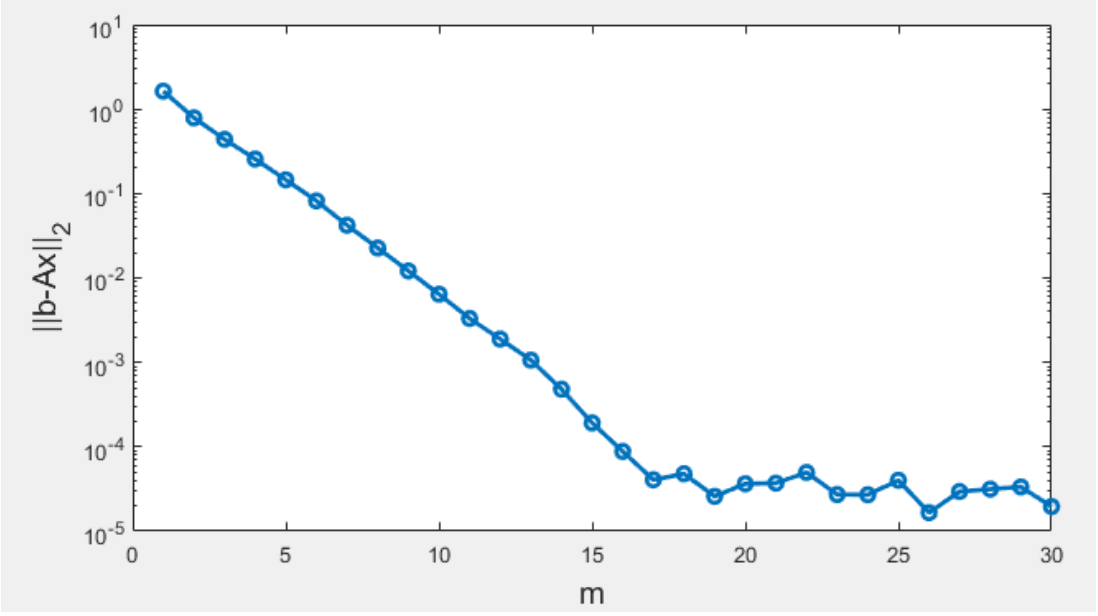
Example 8.4.1

```
% Now we solve a least squares problem for
% Krylov matrices of increasing dimension.
for m = 1:30
    z = ( A*Km(:,1:m) )\b;
    x = Km(:,1:m)*z;
    resid(m) = norm( b-A*x );
end

% The linear system approximations show smooth
% linear convergence at first, but
% the convergence stagnates after only a
% few digits have been found.
semilogy(resid,'o-','LineWidth',2)
ylabel('||b-Ax||_2','FontSize',14)
xlabel('m','FontSize',14)
```

- Use the first m columns of K_m to approximate the solution
- \ does least squares solution here
- Compute and save the residual

Example: Krylov iteration

Example 8.4.1



- Residual "stalls" at m=17
- Matlab throws warnings at that point because K_m is nearly singular
- We need a better approach!

Fixing the problem

- The Krylov matrix we were generating was for $m = 30$ with

$$K_m = \begin{bmatrix} u & Au & A^2u & \cdots & A^{m-1}u \end{bmatrix}$$

- After column 17, any new columns were nearly dependent on the previous ones: warnings for $m \geq 17$
- The opposite of this problem is to use an orthogonal matrix, where the columns are far from dependent
- Try QR factorization:

$$K_m = Q_m R_m = \begin{bmatrix} q_1 & q_2 & \cdots & q_m \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1m} \\ 0 & R_{22} & \cdots & R_{2m} \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & R_{mm} \end{bmatrix}$$

Fixing the problem

- The columns $\boldsymbol{q}_j, j = 1, \ldots, m$ of $\boldsymbol{Q}$ are orthonormal
- And, they are a basis for $\mathcal{K}_m$!
- From Lemma 8.4.1, we know that multiplying a vector in $\mathcal{K}_m$ with $\boldsymbol{A}$ will produce a vector in $\mathcal{K}_{m+1}$
- Using the last column of $\boldsymbol{Q}$, we know that

$$\boldsymbol{A}\boldsymbol{q}_m \in \mathcal{K}_{m+1}$$

- It's then a linear combo of the $m + 1$ columns of another $\boldsymbol{Q}$:

$$A q_m = H_{1m}\, q_1 + H_{2m}\, q_2 + \cdots + H_{m+1,m}\, q_{m+1},$$

Fixing the problem

- Because the columns $\boldsymbol{q}_j$ are orthonormal,

$$\boldsymbol{q}_i^* \boldsymbol{q}_j = 0, \qquad i \neq j$$
$$\boldsymbol{q}_i^* \boldsymbol{q}_j = 1, \qquad i = j$$

- Premultiply by $\boldsymbol{q}_i^*$, and only one term on the right survives:

$$\boldsymbol{q}_i^* \left(A q_m = H_{1m}\, q_1 + H_{2m}\, q_2 + \cdots + H_{m+1,m}\, q_{m+1} \right)$$

- We get $\boldsymbol{q}_i^* \left(\boldsymbol{A} \boldsymbol{q}_j \right) = H_{im}, i = 1, \ldots, m$
- Orthonormality of the $\boldsymbol{q}_j$ makes this easy!!
- The first m $\boldsymbol{q}_j$ are known, and the H_{im} are then determined.
- What about the last term on the right?

Fixing the problem: Arnoldi iteration

- With the first m $\boldsymbol{q}_j$ are known, and the H_{im} found, we can rearrange:

$$H_{m+1,m}\boldsymbol{q}_{m+1} = \boldsymbol{A}\boldsymbol{q}_m - \sum_{i=1}^{m} H_{im}\boldsymbol{q}_i$$

- Now, we only know $H_{m+1,m}\boldsymbol{q}_{m+1}$
- However, we know that we want $\boldsymbol{q}_{m+1}$ to be a *unit vector*
- So, we can make $H_{m+1,m}$ the norm of the result, and make $\boldsymbol{q}_{m+1}$ its direction.
- This is called *Arnoldi iteration*

Arnoldi iteration

- Here's an algorithm

1. Let $q_1 = u/\|u\|$.
2. For $m = 1, 2, \ldots$
   i. Use (8.4.4) to find H_{im} for $i = 1, \ldots, m$.
   ii. Let

$$v = (Aq_m) - H_{1m}\, q_1 - H_{2m}\, q_2 - \cdots - H_{mm}\, q_m.$$

   iii. Let $H_{m+1,m} = \|v\|$.
   iv. Let $q_{m+1} = v/H_{m+1,m}$.

- The big improvement here is that the Arnoldi algorithm finds an orthonormal basis for the Krylov subspace

Example: Arnoldi iteration

Make a few steps of Arnoldi iteration for a small matrix

Example 8.4.2

```
% A few steps of Arnoldi iteration using a small matrix
A = magic(6) ;

% The seed vector determines the first member of the orthonormal basis.
u = randn(6 ,1);
Q = u/norm(u)

% Multiplication by A gives us a new vector in K2.
Aq = A*Q(:,1)

% We subtract off its projection in the previous direction.
% The remainder is rescaled to give us the next orthonormal column.
v = Aq-(Q(:,1)'*Aq)*Q(:,1)
Q(:,2) = v/norm (v)
```

- The first column was the unit vector in the u direction
- The second vector is A times that first vector, then normalized

Example: Arnoldi iteration

Make a few steps of Arnoldi iteration for a small matrix

Example 8.4.2

```
% On the next pass, we have to subtract off
% the projections in two previous directions.
Aq = A*Q(:,2);
v = Aq - (Q(:,1)'*Aq)*Q(:,1) - (Q(:,2)'*Aq)*Q(:,2)
Q(:,3) = v/norm(v)

% At every step, Qm is an ONC matrix.
norm ( Q'*Q - eye(3) )

% And Qm spans the same space as the 3-dimensional Krylov matrix.
K = [ u A*u A*A*u ];
rank ( [Q,K] )
```

```
Q =
   -0.7836   -0.3993    0.0892
    0.2807    0.2386    0.5703
    0.2801   -0.4678    0.0839
    0.1849    0.2795   -0.2166
    0.3077   -0.3680   -0.6645
   -0.3161    0.5927   -0.4138
ans =
   2.5117e-16
ans =
     3
```

A Key Identity

- We focused on the $\boldsymbol{q}_j$ so far, but the H_{im} are important too
- They can be assembled into an *upper Hessenberg* matrix:

$$AQ_m = \begin{bmatrix} Aq_1 & \cdots & Aq_m \end{bmatrix}$$

$$= \begin{bmatrix} q_1 & q_2 & \cdots & q_{m+1} \end{bmatrix} \begin{bmatrix} H_{11} & H_{12} & \cdots & H_{1m} \\ H_{21} & H_{22} & \cdots & H_{2m} \\ & H_{32} & \ddots & \vdots \\ & & \ddots & H_{mm} \\ & & & H_{m+1,m} \end{bmatrix} = Q_{m+1} H_m,$$

- This is a fundamental identity for Krylov subspace methods
- We will study practical and widely used methods based on it

Function 8.4.1 (arnoldi) Arnoldi iteration for Krylov subspaces.

```
function [Q,H] = arnoldi(A,u,m)
% ARNOLDI   Arnoldi iteration for Krylov subspaces.
% Input:
%   A     square matrix (n by n)
%   u     initial vector
%   m     number of iterations
% Output:
%   Q     orthonormal basis of Krylov space (n by m+1)
%   H     upper Hessenberg matrix, A*Q(:,1:m)=Q*H (m+1 by m)

n = length(A);
Q = zeros(n,m+1);
H = zeros(m+1,m);
Q(:,1) = u/norm(u);
for j = 1:m
  % Find the new direction that extends the Krylov subspace.
  v = A*Q(:,j);
  % Remove the projections onto the previous vectors.
  for i = 1:j
    H(i,j) = Q(:,i)'*v;
    v = v - H(i,j)*Q(:,i);
  end
  % Normalize and store the new basis vector.
  H(j+1,j) = norm(v);
  Q(:,j+1) = v/H(j+1,j);
end
```

Section 8.5
GMRES

GMRES: Using Arnoldi iteration

- Arnoldi iteration may be most widely used to solve the square linear system $\boldsymbol{Ax} = \boldsymbol{b}$ for n unknowns $\boldsymbol{x}$
- The Krylov basis (columns of K_m) was bad because some of the basis vectors were nearly dependent
- We tried to solve

$$\min_{\boldsymbol{x}\in\mathcal{K}_m} \|\boldsymbol{Ax} - \boldsymbol{b}\| = \min_{\boldsymbol{z}\in\mathbb{C}^m} \|\boldsymbol{AK}_m\boldsymbol{z} - \boldsymbol{b}\|,$$

- But, we found trouble when m got bigger
- We then went to an orthonormal basis from the QR factorization

$$\boldsymbol{K}_m = \boldsymbol{Q}_m\boldsymbol{R}_m$$

GMRES: Using Arnoldi iteration

- Use the orthonormal columns of as the basis for the approximate answer: $\boldsymbol{x} = \boldsymbol{Q}_m \boldsymbol{z}$ for n unknowns $\boldsymbol{x}$
- Then we have converted the problem to

$$\min_{\boldsymbol{z} \in \mathbb{C}^m} \|\boldsymbol{A}\boldsymbol{Q}_m \boldsymbol{z} - \boldsymbol{b}\|.$$

- At this point, there are n equations for the m coefficients in $\boldsymbol{z}$
- To make the method efficient, we can make the system smaller: use $\boldsymbol{A}\boldsymbol{Q}_m = \boldsymbol{Q}_{m+1}\boldsymbol{H}_m$
- Then we have

$$\min_{\boldsymbol{z} \in \mathbb{C}^m} \|\boldsymbol{Q}_{m+1}\boldsymbol{H}_m \boldsymbol{z} - \boldsymbol{b}\|.$$

GMRES: Using Arnoldi iteration

- This system still has n equations for the m coefficients in $\boldsymbol{z}$

$$\min_{z \in \mathbb{C}^m} \|Q_{m+1} H_m z - b\|.$$

- Note that $\boldsymbol{b}$ is a multiple of the unit vector $\boldsymbol{q}_1$; we can then write

$$\boldsymbol{b} = \big|\|\boldsymbol{b}\|\big| \boldsymbol{Q}_{m+1} \boldsymbol{e}_1$$

- Now substitute for $\boldsymbol{b}$, to get the new problem

$$\min_{z \in \mathbb{C}^m} \|Q_{m+1}(H_m z - \|b\| e_1)\|.$$

- Is this better? It is still n equations for the m coefficients in $\boldsymbol{z}$
- But, for $w \in \mathbb{C}^{m+1}$, we have

$$\|Q_{m+1} w\|^2 = w^* Q_{m+1}^* Q_{m+1} w = w^* w = \|w\|^2.$$

GMRES: Using Arnoldi iteration

- These orthogonal matrices don't change the norm!
- We need only minimize the smaller system without the $\boldsymbol{Q}_{m+1}$

Thus

$$\min_{\boldsymbol{z}\in\mathbb{C}^m} \|\boldsymbol{Q}_{m+1}(\boldsymbol{H}_m\boldsymbol{z} - \|\boldsymbol{b}\|\boldsymbol{e}_1)\|.$$

becomes

$$\min_{\boldsymbol{z}\in\mathbb{C}^m} \|\boldsymbol{H}_m\boldsymbol{z} - \|\boldsymbol{b}\|\boldsymbol{e}_1\|,$$

- Is this better? Now only $(\mathrm{m}+1)$ eqns for the m coefficients in $\boldsymbol{z}$
- The solution for this system is $\boldsymbol{z}_m$
- The solution to the original system is approximately $\boldsymbol{x}_m = \boldsymbol{Q}_m\boldsymbol{z}_m$

GMRES: Using Arnoldi iteration

- This method is called GMRES, for Generalized Minimum RESidual

$$\min_{z \in \mathbb{C}^m} \left\| H_m z - \|b\| e_1 \right\|,$$

$$x_m = Q_m z_m$$

- GMRES uses the output of the Arnoldi iteration to minimize the residual of $Ax = b$ over successive Krylov subspaces.
- Let's look at an example

Example: GMRES

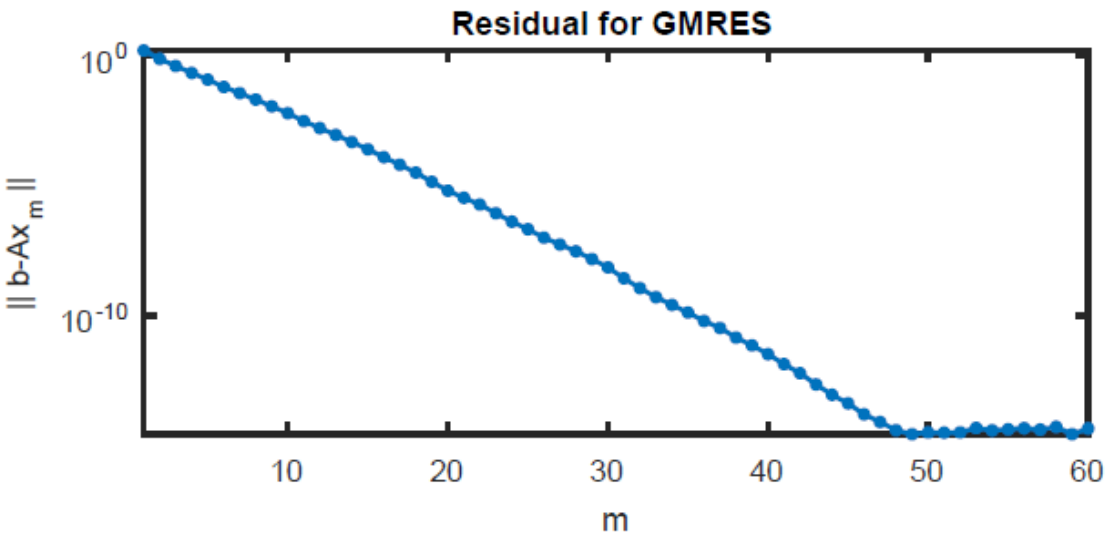
Example 8.5.1

```
lambda = 10 + (1:100);
A = diag(lambda) + triu(rand(100),1);
b = rand(100,1);

[Q,H] = arnoldi(A,b,60);

for m = 1:60
    s = [norm(b); zeros(m,1)];
    z = H(1:m+1,1:m)\s;
    x = Q(:,1:m)*z;
    resid(m) = norm(b-A*x);
 end

semilogy(resid,'.-')
```

- Matrix with known e-values and random ***b***
- K_m not used, created ***Q,H*** instead
- Create a sequence of 60 approximations using one more column each time
- Plot all the residuals

Example: GMRES

Example 8.5.1



- Error drops to nearly machine epsilon before 50 columns
- No stalling of the error here

GMRES

- A basic version of the algorithm is implemented in Function 8.5.1

Function 8.5.1 (arngmres) GMRES for a linear system.

```
1  function [x,residual] = arngmres(A,b,M)
2  % ARNGMRES   GMRES for a linear system (demo only).
3  % Input:
4  %   A       square matrix (n by n)
5  %   b       right-hand side (n by 1)
6  %   M       number of iterations
7  % Output:
8  %   x       approximate solution (n by 1)
9  %   r       history of norms of the residuals
10
11 n = length(A);
12 Q = zeros(n,M);
13 Q(:,1) = b/norm(b);
14 H = zeros(M,M-1);
15
16 % Initial "solution" is zero.
17 residual(1) = norm(b);
18
```

GMRES

- A basic version of the algorithm is implemented in Function 8.5.1

```
18
19  for m = 1:M
20
21    % Next step of Arnoldi iteration.
22    v = A*Q(:,m);
23    for i = 1:m
24        H(i,m) = Q(:,i)'*v;
25        v = v - H(i,m)*Q(:,i);
26    end
27    H(m+1,m) = norm(v);
28    Q(:,m+1) = v/H(m+1,m);
29
30    % Solve the minimum residual problem.
31    r = norm(b)*eye(m+1,1);
32    z = H(1:m+1,1:m) \ r;
33    x = Q(:,1:m)*z;
34    residual(m+1) = norm( A*x - b );
35
36  end
```

- Matlab has a more sophisticated version: `gmres`

GMRES: convergence and restarting

- The residual $||\boldsymbol{r}_m|| = ||\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_m||$ can't increase during Arnoldi iteration because minimization over the largest space includes the previous ones
- But, it is difficult to say more than that.
- The previous example showed the cleanest behavior.
- It turns out that phases of sublinear and superlinear convergence can happen in (typically larger) systems. This depends on the spectrum of the matrix.
- Also, the number of columns of $\boldsymbol{Q}$ and the number of entries in $\boldsymbol{H}_m$: work and storage grow like m^2, which can be too much
- Using GMRESS with *restarting* can help

GMRES: convergence and restarting

- Good things about restarting:
  - one does not lose the previous gain of getting close to the answer
  - one uses low dimensional approximations again so that memory used is never allowed to get too large
- However, the low dimensional approximations may retard or even stagnate progress
- Matlab's GMRES function allows restarting
- Number of restarts (including initial): *outer iterations*
- Number of iterations after restarting: *inner iterations*

Example: GMRES with restarting

Example 8.5.2

```
maxit = 120;  rtol = 1e-8;
d = 50;
A = d^2*gallery('poisson',d);
n = size(A,1)
b = ones(n,1);
```

```
n =
        2500
```

- Matrix discretizing a PDE that will be used not uncommonly
- The name compes from the PDE problem: Poisson equation
- From built-in `gallery` function
- Gives a large matrix

Example: GMRES with restarting

Example 8.5.2

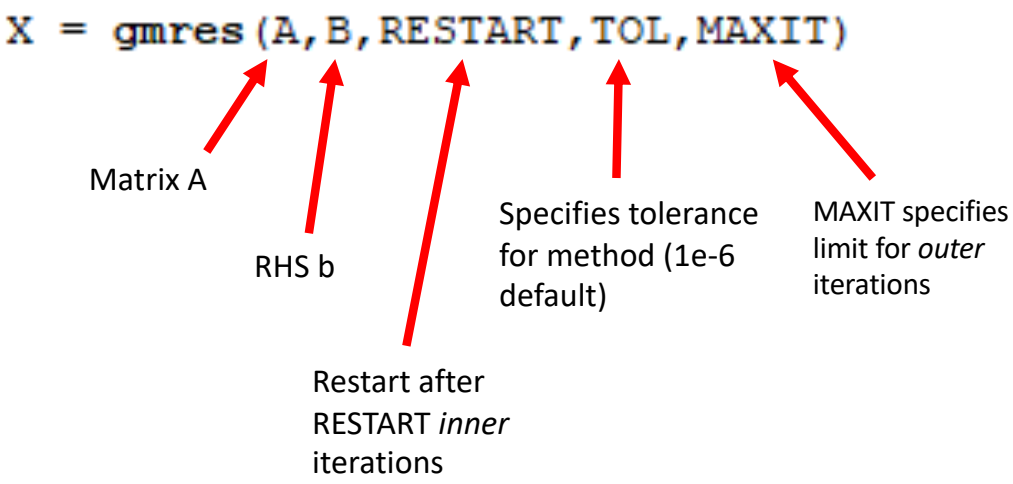
- We use these five input arguments

```
>> help gmres
 gmres   Generalized Minimum Residual Method.
    X = gmres(A,B) attempts to solve the system of linear equations A*X = B
    for X.  The N-by-N coefficient matrix A must be square and the right
    hand side column vector B must have length N. This uses the unrestarted
    method with MIN(N,10) total iterations.

    X = gmres(A,B,RESTART) restarts the method every RESTART iterations.
    If RESTART is N or [] then gmres uses the unrestarted method as above.

    X = gmres(A,B,RESTART,TOL) specifies the tolerance of the method.  If
    TOL is [] then gmres uses the default, 1e-6.

    X = gmres(A,B,RESTART,TOL,MAXIT) specifies the maximum number of outer
    iterations. Note: the total number of iterations is RESTART*MAXIT. If
    MAXIT is [] then gmres uses the default, MIN(N/RESTART,10). If RESTART
    is N or [] then the total number of iterations is MAXIT.
```

Example: GMRES with restarting

Example 8.5.2

- We use these five input arguments



Example: GMRES with restarting

Example 8.5.2

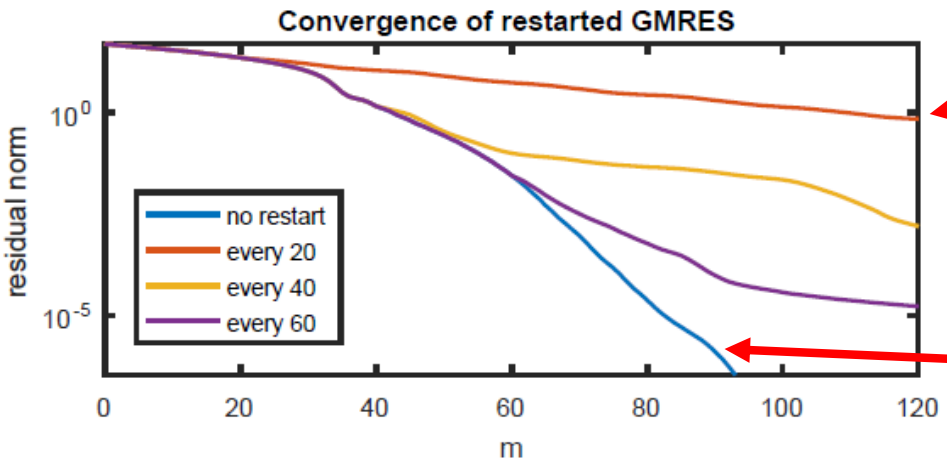
```
[X,FLAG,RELRES,ITER,RESVEC] = gmres(A,B,...) also returns a vector of
the residual norms at each inner iteration, including NORM(B-A*X0).
Note with preconditioners M1,M2, the residual is NORM(M2\(M1\(B-A*X))).
```

- We use only the last of these five outputs here
- X is approximate answer is X
- RELRES gives relative residual of X, ||B-A*X||/||B||
- FLAG states whether we achieved the tolerance
- ITER returns the outer and inner iteration number of the solution
- RESVEC is the list of residual values over iterations ||B-A*X||

Example: GMRES with restarting

Example 8.5.2

```
rest = [maxit 20 40 60];
for j = 1:4
    [~,~,~,~,rv] = gmres(A,b,rest(j),rtol,maxit/rest(j));
    semilogy(0:length(rv)-1,rv,'-'), hold on
end
```



- Most restarts: GMRES had not got to rapidly converging part before restart
- No restarts

GMRES: comments

- There are a lot of variations for solving $\boldsymbol{Ax} = \boldsymbol{b}$ using Krylov based methods
- These include
  - QMR: quasi-minimal residual
  - CGS: conjugate gradient stabilized
  - BiCGStab: bi-conjugate gradient stabilized
  - And more…
- We will discuss two special cases in the next section

Section 8.6
MINRES and conjugate gradients

Special cases of GMRES

- Some really nice simplifications can be made in special cases of solving $\boldsymbol{Ax} = \boldsymbol{b}$, depending on the properties of $\boldsymbol{A}$
- Consider Hermitian $\boldsymbol{A}$, where $\boldsymbol{A}^* = \boldsymbol{A}$
- For square systems, we know that $\boldsymbol{AQ}_m = \boldsymbol{Q}_{m+1}\boldsymbol{H}_m$
- Use the nice properties of an orthogonal matrix: pre-multiply by $\boldsymbol{Q}_m^*$ to get

$$Q_m^* A Q_m = Q_m^* Q_{m+1} H_m = \widetilde{H}_m,$$

- $\widetilde{H}_m$ is first m rows of $\boldsymbol{H}_m$, and it's Hessenberg form
- The lhs is Hermitian; the rhs must be too: $\widetilde{\boldsymbol{H}}_m$ is tridiagonal!

Special cases of GMRES: MINRES

- This is news we can use!
- The Arnoldi iteration has only a few components at each step:

$$A\boldsymbol{q}_m = H_{m-1,m}\,\boldsymbol{q}_{m-1} + H_{mm}\,\boldsymbol{q}_m + H_{m+1,m}\,\boldsymbol{q}_{m+1}.$$

- We only need to find $H_{m-1,m}$, H_{mm}, $H_{m-1,m}$, $\boldsymbol{q}_{m+1}$
- This truncated version of Arnoldi iteration is called *Lanczos iteration*
- Perhaps the best thing about this is that we need only a couple of previous vectors and a few coefficients each step
- This is only O(1) steps per iteration: No need for restarts!

MINRES

- Matlab has a built-in function `minres`
- It also is relatively tractable for convergence analysis.
- If A is hermitian, then it has real eigenvalues
- Let $s_+ = \{\lambda_i | \lambda > 0\}$ and define $\kappa_+ = \max \lambda_i \,/\, \min \lambda_i$
- Let $s_- = \{\lambda_i | \lambda < 0\}$ and define $\kappa_- = \min \lambda_i \,/\, \max \lambda_i$

$$\frac{\|\boldsymbol{r}_m\|_2}{\|\boldsymbol{b}\|_2} \leq \left(\frac{\sqrt{\kappa_+ \kappa_-} - 1}{\sqrt{\kappa_+ \kappa_-} + 1} \right)^{\lfloor m/2 \rfloor},$$

- $\lfloor m/2 \rfloor$ is the floor function (round $m/2$ down to nearest integer)
- If $\kappa_+ \kappa_-$ is large, the ratio inside the parens tends to unity, and the convergence is slow

MINRES

- Matlab has a built-in function `minres`
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- Let $s_- = \{\lambda_i | \lambda < 0\}$ and define $\kappa_- = \min \lambda_i \,/\, \max \lambda_i$

$$\frac{\|\boldsymbol{r}_m\|_2}{\|\boldsymbol{b}\|_2} \leq \left(\frac{\sqrt{\kappa_+ \kappa_-} - 1}{\sqrt{\kappa_+ \kappa_-} + 1} \right)^{\lfloor m/2 \rfloor},$$

- $\lfloor m/2 \rfloor$ is the floor function (round $m/2$ down to nearest integer)
- If $\kappa_+ \kappa_-$ is large, the ratio inside the parens tends to unity, and the convergence is slow

The conjugate gradient method

- Let's specify that nonsingular $\boldsymbol{A}$ from $\boldsymbol{Ax} = \boldsymbol{b}$ is HPD
- Then $\boldsymbol{A}$ has a Cholesky factorization: $\boldsymbol{A} = \boldsymbol{R}^*\boldsymbol{R}$
- For any vector u, we have

$$u^*Au = (Ru)^*(Ru) = \|Ru\|^2,$$

- This is great because it is non-negative, and zero iff $\boldsymbol{u} = \boldsymbol{0}$
- We can then define

$$\|u\|_{\boldsymbol{A}} = (u^*Au)^{1/2}.$$

- The conjugate gradient method minimizes the error measured with the A-norm over the sequence of Krylov subspaces
- That is, it computes $\min_{\mathcal{K}_m} \left|\left|x_m - x\right|\right|_A$

The conjugate gradient method

- The conjugate gradient (CG) computes directions for each iterate that are “A-orthogonal” and estimates how long they should be.
- Another take on CG based on this view on the Sakai site
- It began being designed for n steps, i.e., as a direct method, but suffered from the same problem as Krylov iteration.
- Only later did it become a useful iterative method.
- The classical CG method is somewhat limited by the need for an HPD matrix
- But, that same list of modified functions applied to the CG method
- Matlab has a built-in function `pcg`

Convergence of MINRES and CG

- Let $\boldsymbol{A}$ be real and nonsingular with $\kappa = \left|\left|A^{-1}\right|\right|_2 \left|\left|A\right|\right|_2$
- We have the following theorem:

Theorem 8.6.1

Let $\boldsymbol{A}$ be real and SPD with 2-norm condition number κ. For MINRES define $R(m) = \|r_m\|_2/\|b\|_2$, and for CG define $R(m) = \|x_m - x\|_{\boldsymbol{A}}/\|x\|_{\boldsymbol{A}}$, where r_m and x_m are the residual and solution approximation associated with the space $\mathcal{K}_m$. Then

$$R(m) \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^m. \qquad (8.6.4)$$

- MINRES: bound on *relative residual*; CG: on *relative error*
- If κ is large, convergence is slow: spectrum of $\boldsymbol{A}$ matters!
- Bigger exponent than indefinite case

Convergence of MINRES and CG

- Using this result, we can estimate how many steps are needed.
- Let κ be a parameter (i.e., given)
- We want to specify a tolerance, say ε; to get the bound under this value, we need $2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^m \approx \epsilon$
- Solve for m: $m \log\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right) \approx \log\left(\frac{\epsilon}{2}\right).$
- Simplify assuming large κ:

$$\begin{aligned}\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} &= (1-\kappa^{-1/2})(1+\kappa^{-1/2})^{-1} \\ &= (1-\kappa^{-1/2})(1-\kappa^{-1/2}+\kappa^{-1}+\cdots) \\ &= 1-2\kappa^{-1/2}+O(\kappa^{-1}), \quad \text{as } \kappa \to \infty.\end{aligned}$$

Convergence of MINRES and CG

- Now use the last result inside the log function and Taylor expand to get

$$\log(1+x) = x - (x^2/2) + \cdots,$$

- Finally, we obtain

$$-2m\kappa^{-1/2} \approx \log\left(\frac{\epsilon}{2}\right), \text{ or } m = O(\sqrt{\kappa}),$$

- It is easy to see that the number of iterations m increases with $\kappa^{1/2}$ and with decreasing tolerance ε
- Let's do an example

Example: MINRES and CG

Example 8.6.1

```
n = 1000;
density = 0.008;
A = sprandsym(n,density,1e-2,2);
x = (1:n)'/n;
b = A*x;
```

- Create sparse random matrix
- Condition number 100
- Known solution

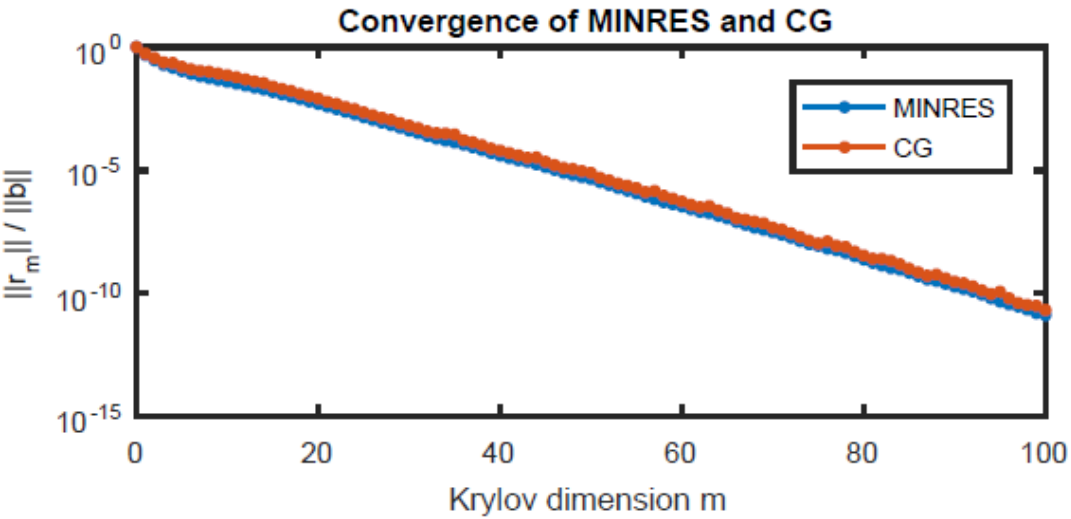
```
[xMR,~,~,~,residMR] = minres(A,b,1e-12,100);
[xCG,~,~,~,residCG] = pcg(A,b,1e-12,100);
semilogy(0:100,residMR/norm(b),'.-')
hold on, semilogy(0:100,residCG/norm(b),'.-')
```

- `minres` used first
- `pcg` second
- Same tolerance
- Plot relative residuals

Example: MINRES and CG

Example 8.6.1

```
[xMR,~,~,~,residMR] = minres(A,b,1e-12,100);
[xCG,~,~,~,residCG] = pcg(A,b,1e-12,100);
semilogy(0:100,residMR/norm(b),'.-')
hold on, semilogy(0:100,residCG/norm(b),'.-')
```



- `minres` and `pcg` residuals are very similar here
- What about error?
- We know exact solution here

Example: MINRES and CG

Example 8.6.1

```
errorMR = norm( xMR - x ) / norm(x)
errorCG = norm( xCG - x) / norm(x)
```

```
errorMR =
   1.1192e-10
errorCG =
   7.9932e-11
```

```
A = sprandsym(n,density,1e-4,2);
```

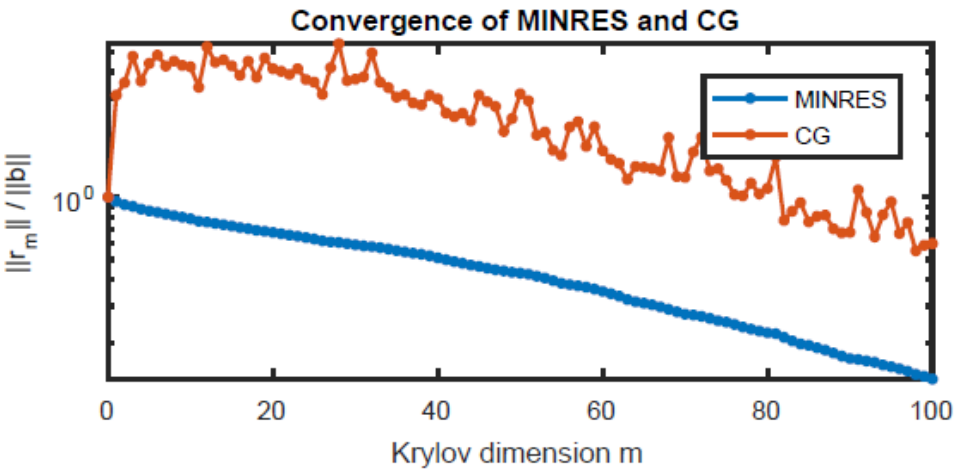
- Using the exact solution, we little difference when the condition number is $\kappa = 100$

- Now let's up the ante and use a condition number of $\kappa = 10^4$

Example: MINRES and CG

Example 8.6.1

```
[xMR,~,~,~,residMR] = minres(A,b,1e-12,100);
[xCG,~,~,~,residCG] = pcg(A,b,1e-12,100);
clf
semilogy(0:100,residMR/norm(b),'.-')
hold on, semilogy(0:100,residCG/norm(b),'.-')
```



- `minres` and `pcg` residuals' decay *rates* are similar, but residual bigger for CG
- Very little progress toward answer
- What about error?

Example: MINRES and CG

Example 8.6.1

```
errorMR = norm( xMR - x ) / norm(x)
errorCG = norm( xCG - x) / norm(x)
```

```
errorMR =
  922.3604
errorCG =
   1.0061e+03
```

- Yep, that error is bad!
- Theory: $\kappa = 100$, $2\left(\frac{9}{11}\right)^{100} \approx 3.9\times10^{-9}$
- Theory: $\kappa = 10^4$, $2\left(\frac{99}{101}\right)^{100} \approx 0.27$
- Larger κ has strong effect!

$$R(m) \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^m$$

About stopping criteria

- $\boldsymbol{Ax} = \boldsymbol{b}$; in mth iteration is $\boldsymbol{x}_m$; $\boldsymbol{r}_m = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_m$
- We can think of solution as $\boldsymbol{x} = \boldsymbol{x}_m + \boldsymbol{\delta}_m$
- Substitution gives $\boldsymbol{A}(\boldsymbol{x}_m + \boldsymbol{\delta}_m) = \boldsymbol{b}$, or $\boldsymbol{A}\boldsymbol{\delta}_m = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_m = \boldsymbol{r}_m$
- Approximately solving $\boldsymbol{A}\boldsymbol{\delta}_m = \boldsymbol{r}_m$ for the "correction" gives us an updated solution $\boldsymbol{x}_{m+1} = \boldsymbol{x}_m + \boldsymbol{\delta}_m$
- Iteration can be stopped when $||\boldsymbol{\delta}_m||$ or $||\boldsymbol{r}_m||$, or both, are smaller than preset tolerances
- When A is ill-conditioned, $||\boldsymbol{r}_m||$ may be very small, while $||\boldsymbol{\delta}_m||$ isn't: be careful

$$\frac{\|x - \tilde{x}\|}{\|x\|} \leq \kappa(A)\frac{\|r\|}{\|b\|}. \qquad (2.8.4)$$

Section 8.7
Matrix-free Iterations

Linear transformations, and undoing them

- We can think of $\boldsymbol{Ax} = \boldsymbol{b}$ as a linear transformation of $\boldsymbol{x}$ to $\boldsymbol{b}$
- The solution process undoes this transformation, $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$
- Interestingly, we can undo a linear transformation without having to explicitly form the matrix $\boldsymbol{A}$!
- How can we do this? Let's try an example.

Linear transformations, and undoing them

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- Interestingly, we can undo a linear transformation without having to explicitly form the matrix $\boldsymbol{A}$!
- How can we do this? Let's try an example.

Blurring images

- We can think of an image as an $m \times n$ matrix $\boldsymbol{X}$, as we've already done
- Let's consider a simple model process for blurring
- Let the tridiagonal $m \times n$ matrix $\boldsymbol{B}$ be given by

$$B_{ij} = \begin{cases} \frac{1}{2}, & \text{if } i = j \\ \frac{1}{4}, & \text{if } |i - j| = 1 \\ 0, & \text{otherwise.} \end{cases}$$

- Pre-multiplication forms weighted combos or averages of elements in each column: $\boldsymbol{BX}$
- This smears column elements

Blurring images

- For rows, we can make a matrix with elements as it B, but make it $n \times n$
- Call this tridiagonal matrix $\boldsymbol{C}$
- We can accomplish row blurring with transposes

$$(CX^T)^T = XC^T = XC$$

- We can get blurring of both rows and columns with

$$\text{blur}(X) = B^k X C^k$$

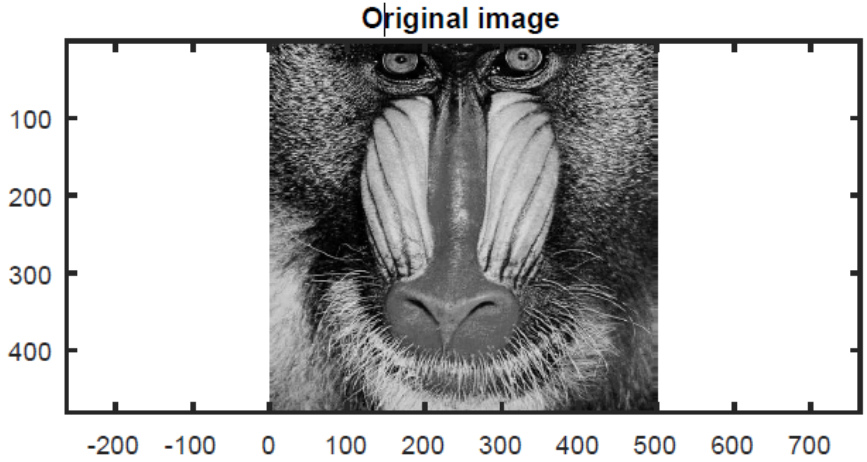
- Integer $k \geq 1$

Blurring example

Example 8.7.1

```
load mandrill
[m,n] = size(X)
image(X), colormap(gray(256))
```

```
m =
   480
n =
   500
```



- We use our best old ex-friend the mandrill
- Now make some blurring matrices, and combine them for a blur function

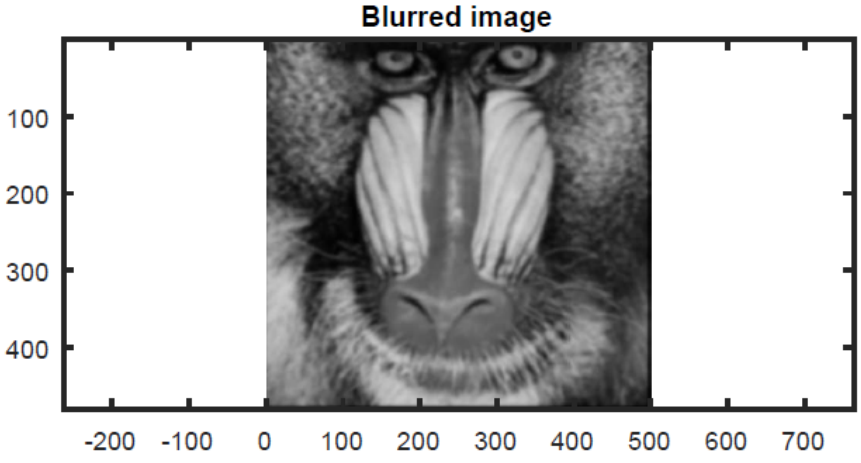
```
v = [1/4 1/2 1/4];
B = spdiags( repmat(v,m,1), -1:1, m,m);
C = spdiags( repmat(v,n,1), -1:1, n,n);

blur = @(X) B^12 * X * C^12;
```

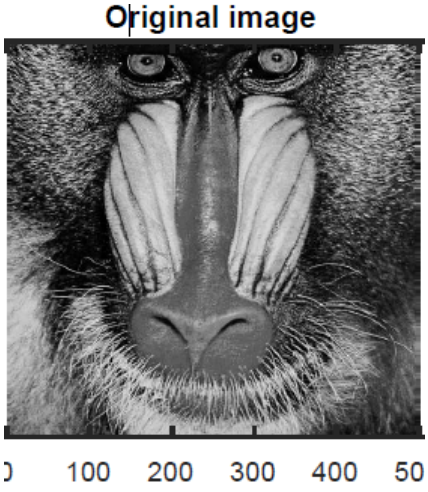
Blurring example

Example 8.7.1

This is what the blur did at left

```
image(blur(X))
```





Deblurring images

- An important task is to try to deblur poorly focused images
- One way to treat this process is as linear transformation of the image
- To facilitate this, covert the $m \times n$ matrix $\boldsymbol{X}$ to an $mn \times 1$ vector $\boldsymbol{x}$
- Denote this by vec($\boldsymbol{X}$)= $\boldsymbol{x}$
- Converting from vector to matrix will be unvec($\boldsymbol{x}$)= $\boldsymbol{X}$
- We use blurring process from before $\boldsymbol{Z}$ = blur($\boldsymbol{X}$)

Deblurring images

- Because the blurring is a linear transformation, we can write it as $\boldsymbol{A}\,\mathrm{vec}(\boldsymbol{X}) = \mathrm{vec}(\boldsymbol{Z})$.
- The matrix A is $mn \times mn$
- For a 12 megapixel image, 1.4×10^4 entries!!!
- The matrix is very sparse but it is not necessary
- Given an input vector $\boldsymbol{u}$, we can compute $\boldsymbol{v} = \boldsymbol{A}\boldsymbol{u}$ via

$$\begin{aligned} \boldsymbol{U} &= \mathrm{unvec}(\boldsymbol{u}) \\ \boldsymbol{V} &= \mathrm{blur}(\boldsymbol{U}) \\ \boldsymbol{v} &= \mathrm{vec}(\boldsymbol{V}). \end{aligned}$$

- Our blur recipe can be used without constructing $\boldsymbol{A}$

Deblurring example

Example 8.7.2

```
load mandrill
[m,n] = size(X)
v = [1/4 1/2 1/4];
B = spdiags( repmat(v,m,1), -1:1, m,m);
C = spdiags( repmat(v,n,1), -1:1, n,n);
blur = @(X) B^12 * X * C^12;
Z = blur(X);
```

```
m =
   480
n =
   500
```

```
vec = @(X) reshape(X,m*n,1);
unvec = @(x) reshape(x,m,n);
T = @(x) vec( blur(unvec(x)) );
```

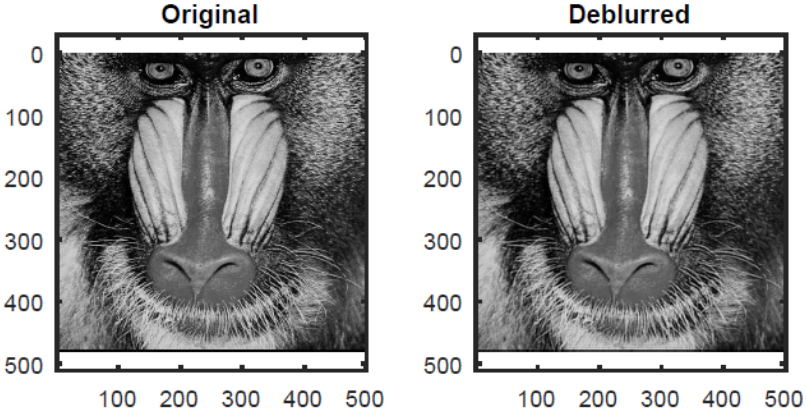
- Mandrill again
- Imagine blurred image Z is given and we want to get back unblurred version X
- Make vec, unvec and blur
- T defines the action of the matrix A but does not create it

Deblurring example

Example 8.7.2

```
y = gmres(T,vec(Z),50,1e-5);
Y = unvec(y);
subplot(121)
image(X), colormap(gray(256))
subplot(122)
image(Y), colormap(gray(256))
```

```
gmres(50) converged at outer iteration 2 (inner iteration
    45) to a solution with relative residual 1e-05.
```



- Apply GMRES to finding the inverse of the blur transformation
- The function T is passed in rather than the matrix: this effective says how to compute the matrix vector produce $\boldsymbol{Au}$
- Not a perfect deblurring

Section 8.8
Preconditioning

Preconditioning

- As condition number increases, convergence of Krylov methods deteriorates
- Preconditioning can help get around this
- Say we are solving $\boldsymbol{Ax} = \boldsymbol{b}$
- The idea is to use an easily inverted matrix that is close the original $\boldsymbol{A}$ that gives a better conditioned system
- Say we are choosing $\boldsymbol{M}$
- Then we are trying to find it so that $(\boldsymbol{M}^{-1}\boldsymbol{A})\boldsymbol{x} = (\boldsymbol{M}^{-1}\boldsymbol{b})$ is easier to solve
- Do we compute $\boldsymbol{M}^{-1}$? NO!!!!!!

Preconditioning

- We want $\boldsymbol{M}$ so that $(\boldsymbol{M}^{-1}\boldsymbol{A})\boldsymbol{x} = (\boldsymbol{M}^{-1}\boldsymbol{b})$ is easier to solve
- Instead of $\boldsymbol{M}^{-1}$, we do the following two step process to compute any $\boldsymbol{y} = (\boldsymbol{M}^{-1}\boldsymbol{A})\boldsymbol{v}$

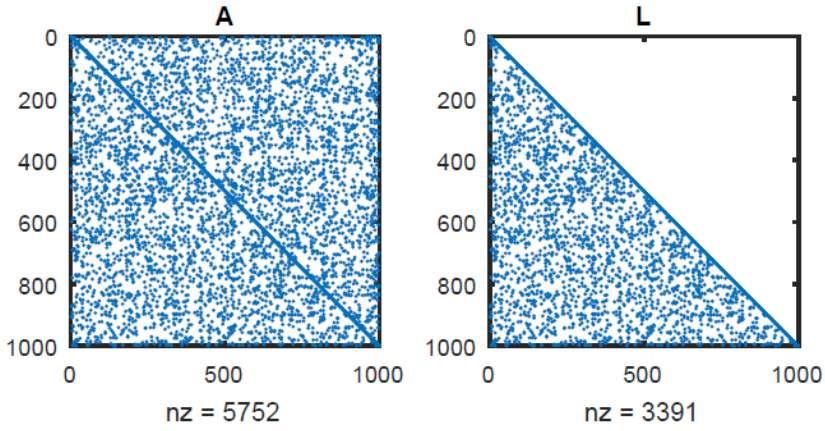
1. Set $\boldsymbol{u} = \boldsymbol{A}\boldsymbol{v}$.
2. Solve $\boldsymbol{M}\boldsymbol{y} = \boldsymbol{u}$ for $\boldsymbol{y}$.

- We use a numerical solve which is more efficient than inverting a matrix
- How to get $\boldsymbol{M}$? One approach is *incomplete LU factorization*, or ILU factorization

Preconditioning: ILU

- We know that LU factorization can ruin sparsity
- ILU says to only save nonzero elements that are similar to the original matrix
- Alternatively, one can set threshold and set to zero any element smaller than that

```
[L,U] = ilu(A);
subplot(121), spy(A)
subplot(122), spy(L)
```

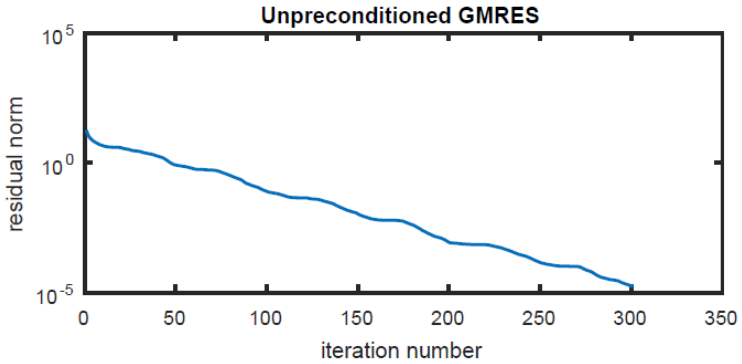


Preconditioning example

Example 8.8.1

Here is a 1000×1000 matrix of density around 0.5%.

```
A = 0.6*speye(1000) + sprand(1000,1000,0.005,1/10000);

b = rand(1000,1);
[x,~,~,resid_plain] = gmres(A,b,50,1e-10,6);  % restart
    at 50
clf, semilogy(resid_plain,'-')
```

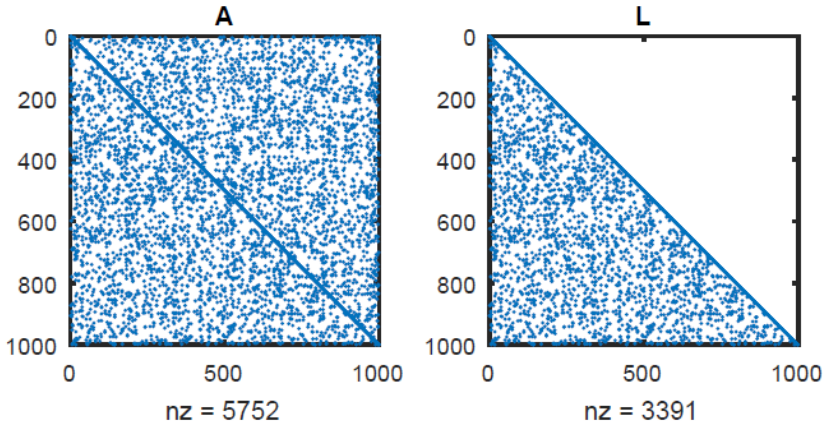


- Slow convergence for this system

Preconditioning example

Example 8.8.1

```
[L,U] = ilu(A);
subplot(121), spy(A)
subplot(122), spy(L)
```



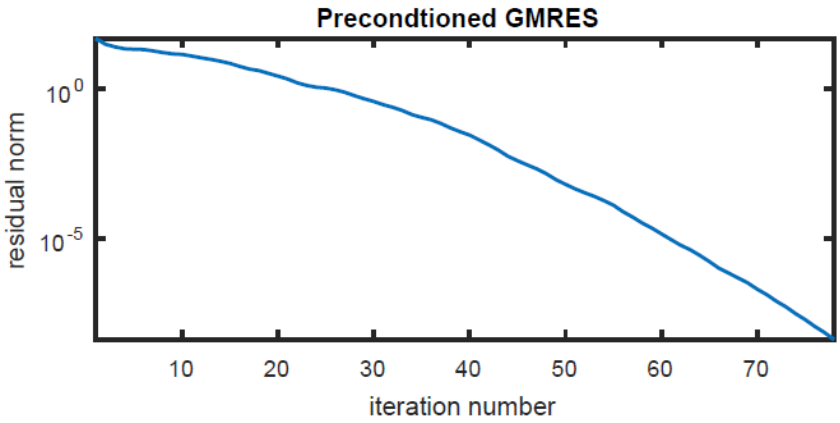
It does *not* produce a true factorization of A.

```
norm( full(A - L*U) )
```

Preconditioning example

Example 8.8.1

```
[x,~,~,~,resid_prec] = gmres(A,b,[],1e-10,300,L,U);
clf, semilogy(resid_prec,'-')
```



- Better now

Preconditioning

- We want $\boldsymbol{M}$ so that $(\boldsymbol{M}^{-1}\boldsymbol{A})\boldsymbol{x} = (\boldsymbol{M}^{-1}\boldsymbol{b})$ is easier to solve
- Not always easy to find
- Our last example found $\boldsymbol{M} = \boldsymbol{LU}$
- If we were doing this manually we would need to solve $(\boldsymbol{M}^{-1}\boldsymbol{b}) = \boldsymbol{c}$, or c = U\(L\b) to get the rhs
- Then use our previous two-step procedure to solve the preconditioned system

1. Set $\boldsymbol{u} = \boldsymbol{Av}$.
2. Solve $\boldsymbol{My} = \boldsymbol{u}$ for $\boldsymbol{y}$.